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Report Title

Development of a Non-Linear Finite Element Code for the Improvement of Piezoelectric Actuator Design and Reliability

ABSTRACT

Chad Landis and Christopher Lynch have developed a finite element code capable of handling constitutive laws with ferroelectric/ferroelastic major hysteresis loops. Two approaches have been developed and compared, a scalar electric field potential based and a vector electric displacement potential based formulation. The code has been used to conduct simulations of geometries in which the field distribution is inhomogeneous and results in local consentrations such as for interdigitated electrodes, for cofired actuators, and for end constraints. Related work on fracture mechanics of ferroelectrics has been completed in parallel with the code development.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

J. Wang and C.M. Landis, 2006. “Effects of In-Plane Electric Fields on the Toughening Behavior of Ferroelectric Ceramics”, to appear in Journal of Mechanics of Materials and Structures.

J. Wang and C.M. Landis, 2006. “Domain Switch Toughening in Polycrystalline Ferroelectrics”, Journal of Materials Research, 21, 13-20.

Oates, W.S., Lynch, C.S. “Orthotropic rescaling for crack tip fields in linear piezoelectric materials”, International Journal of Solids and Structures 41 (11-12) pp 2899-2917 (2003)

Oates, William S.; Lynch, Christopher S.; Lupascu, Doru C.; Njiwa, Alain B. Kounga; Aulbach, Emil; Rodel, Jurgen “subcritical crack growth in lead zirconate titanate” Journal of the American Ceramic Society, v 87, n 7, July, 2004, p 1362-1364A.

Liu, Teiqi; Oates, William S.; Wan, Shan; Lynch, Christopher S. “Crack initiation at electrode edges in PZN-4.5%PT single crystals” Journal of Intelligent Material Systems and Structures, v 16, n 2, February, 2005, p 373-379

Oates, William S.; Lynch, Christopher S.; Kounga Njiwa, Alain B.; Lupascu, Doru C. “Anisotropic fracture behavior in ferroelectric relaxor PZN-4.5%PT single crystals” Journal of the American Ceramic Society, v 88, n 7, July, 2005, p 1838-1844

Landis, C.M., 2004. “Nonlinear constitutive modeling of ferroelectrics”, Current Opinion in Solid State and Materials Science, v. 8, p. 59-69.

Wang, J, Landis, C.M. “On the Fracture Toughness of Ferroelectric Ceramics with Electric Field Applied Parallel to the Crack Front,” Acta Materialia, v. 52, p. 3435-3446.

Landis, C.M., Wang, J., Sheng, J., 2004. “Micro-electromechanical Determination of the Possible Remanent Strain and Polarization States in Polycrystalline Ferroelectrics and the Implications for Phenomenological Constitutive Theories,” J. Int. Mat. Sys. Struct., v. 15, p. 513-525.

Oates, W.S.; Lynch, C.S. "New approach to solving crack tip stress fields for piezoelectric materials" Journal of Intelligent Material Systems and Structures, v 15, n 7, July 2004, p 557-63

Oates, W.S. "Heterogeneity influence on electric field induced piezoelectric microfracture" Journal of Intelligent Material Systems and Structures, v 16, n 9, Sept. 2005, p 733-41

C.M. Landis, 2003. “On the Fracture Toughness of Ferroelastic Materials”, Journal of the Mechanics and Physics of Solids, 51, 1347-1369.

C.M. Landis, 2003. “On the Strain Saturation Conditions for Polycrystalline Ferroelastic Materials”, Journal of Applied Mechanics, 70, 470-478.

Number of Papers published in peer-reviewed journals: 13.00

(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

1. Lynch, C.S. with W.S. Oates "Orthotropy rescaling for the fracture problem in anisotropic piezoelectric materials" American Society of Mechanical Engineers, Aerospace Division (Publication) AD, v 67, 2002, p 97-102
2. Lynch, C.S. with W.S. Oates, "New Approach to Solving Crack Tip Stress Fields for Piezoelectric Materials" Proceedings of SPIE – The International Society for Optical Engineering, v 5053, 2003, p 376-386
3. Lynch, C.S. "Constitutive behavior of ferroelectric materials", Mechamat May 2003, Frejus, France
4. Lynch, C.S. with Oates "Fracture behavior of ferroelectric materials" American Society of Mechanical Engineers, Aerospace Division (Publication) AD 2003
5. Lynch, C.S. with W.S. Oates, "Fracture behavior of Ferroelectric Materials" SPIE March 2004
6. Oates, W.S.; Malbec, A.; Herdic, S.L.; Lynch, C.S. "Phase field modeling of domain structures in ferroelectric materials" Proceedings of the SPIE - The International Society for Optical Engineering, v 5387, n 1, 2004, p 314-25
7. Oates, William S.; Webber, Kyle G.; Lynch, Christopher S.; Njiwa, Alain B. Kounga; Lupascu, Doru C. "Local fracture properties in ferroelectric relaxor PZN-4.5%PT single crystals" Proceedings of SPIE - The International Society for Optical Engineering, v 5761, Smart Structures and Materials 2005 - Active Materials: Behavior and Mechanics, 2005, p 299-304
8. Landis, C.M. 2004. "Nonlinear Fracture Mechanics for Ferroelastic Materials," Proc. SPIE: Smart Materials and Structures, v. 5387, p.326-336.
9. J. Wang and C.M. Landis, 2005. "On the Fracture Toughness of Ferroelectric Ceramics with Electric Field Applied Parallel to the Crack Front", Proceedings of the ICF11.
10. C.M. Landis and J. Wang. "Domain Switch Toughening of Polycrystalline Ferroelectrics", MRS Proceedings, Spring 2005, San Francisco, CA.
11. J. Wang and C.M. Landis, 2005. "Toughening behavior of ferroelectric ceramics under different poling directions", Proceedings of the SPIE, 5761, 305-315.

Number of Papers published in non peer-reviewed journals: 11.00

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

(d) Manuscripts

Number of Manuscripts: 0.00

Number of Inventions:

Graduate Students

NAME	PERCENT_SUPPORTED	
William Oates	0.33	No
Jianxin Wang	1.00	No
FTE Equivalent:	**1.33**	
Total Number:	**2**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Christopher S. Lynch	0.08	No
Chad M. Landis	0.08	No
FTE Equivalent:	**0.16**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Personnel receiving masters degrees

NAME	
William Oates	No
Total Number:	**1**

Names of personnel receiving PHDs

NAME	
William Oates	No
Jianxin Wang	No
Total Number:	**2**

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

The specific aims of this research program were the development of constitutive laws for the nonlinear behavior of ferroelectric ceramics, their incorporation into a finite element code, and the implementation of the code for the analysis of ferroelectric devices including effects of field inhomogeneities that occur due to geometric effects such as flaws, cracks, and partial electrodes.

Initial investigations were performed on purely ferroelastic behavior. A phenomenological constitutive law was developed for the deformation of polycrystalline ferroelastic materials. A model was framed within a thermodynamic setting common to internal variable plasticity. The two significant inputs to this model are a switching (yield) surface, and a hardening potential. To maintain simplicity, the shape of the switching surface was assumed to be spherical in a modified deviatoric stress space. In order to ascertain the functional form of the hardening potential, micromechanical self-consistent simulations of multiple single crystals, with tetragonal crystal structure, embedded in an effective polycrystalline matrix, were performed for differing loading paths in remanent (plastic) strain space. As a result of the asymmetry in the tension versus compression behavior of these materials, it was shown that pure shear loading does not result in pure shear straining. This feature of the material behavior is demonstrated with the self-consistent simulations and predicted by the phenomenological constitutive law. Ultimately, the phenomenological theory is able to capture the complex constitutive behavior of ferroelastic materials predicted by the micromechanical model. Results of this investigation are published in, Landis, C.M., 2003, On the strain saturation conditions for polycrystalline ferroelastic materials, *Journal of Applied Mechanics*, **70**, 470-478.

This new phenomenological constitutive law for ferroelasticity was then used to investigate fracture in ferroelastic materials. In order to perform these fracture investigations A backward Euler integration routine was devised for the constitutive law and implemented within a finite element code. The toughness enhancement due to domain switching near a steadily growing crack in a ferroelastic material was analyzed. The constitutive response of the material was taken to be characteristic of a polycrystalline sample assembled from randomly oriented tetragonal single crystal grains. The constitutive law accounts for the strain saturation, asymmetry in tension versus compression, Bauschinger effects, reverse switching, and strain reorientation that can occur in these materials due to the non-proportional loading that arises near a propagating crack. Crack growth was assumed to proceed at a critical level of the crack tip energy release rate. Detailed finite element calculations were carried out to determine the stress and strain fields near the growing tip, and the ratio of the far field applied energy release rate to the crack tip energy release rate. The results of the finite element calculations were then compared to analytical models that assume the linear isotropic K-field solution holds for either the near tip stress or strain field. Ultimately, the model was able to account for the experimentally observed toughness enhancement in ferroelastic ceramics. The results of this investigation are published in, Landis, C.M., 2003, On the fracture toughness of ferroelastic materials, *Journal of the Mechanics and Physics of Solids*, **51**, 1347-1369.

Preliminary investigations on the electromechanically coupled polarization and strain saturation states in ferroelectric ceramics were performed. The micro-electromechanical constitutive model for polycrystalline ferroelectric ceramics developed by Huber et al. (1999) was implemented to determine the remanent strain and remanent polarization states that are possible in a ferroelectric polycrystal. The underlying crystal structure of the single crystals is assumed to be tetragonal, but the methods developed can be applied to other crystal structures as well. The full multi-axial set of remanent strain saturation states possible in an untextured polycrystal was determined. It was argued and demonstrated that the remanent polarization saturation level is dependent on the prevailing remanent strain state. The possible uniaxial combinations of remanent strain and polarization were determined from the micro-electromechanical model. The results of these investigations were then applied within the phenomenological constitutive framework developed previously by the Landis and the constitutive response under coupled electromechanical loading was predicted. The results of this investigation were published in, C.M. Landis, J. Wang and J. Sheng, 2004. "Micro-electromechanical Determination of the Possible Remanent Strain and Polarization States in Polycrystalline Ferroelectrics and Implications for Phenomenological Constitutive Theories", *Journal of Intelligent Material Systems and Structures,* **15**, 513-525. This paper was also presented at the 2003 SPIE Smart Structures and Materials Conference and has appeared in the proceedings as, Landis, Wang and Sheng, 2003, *Proceedings of the SPIE*, **5053**, 335-346.

Investigations on orthotropy rescaling techniques for the solution of linear piezoelectric boundary value problems were performed. Analysis of stress fields in a linear elastic-piezoelectric-dielectric medium requires use of anisotropic elasticity theory. Many researchers employ the Stroh formalism, which requires the solution of a sixth order characteristic equation involving material coefficients. This equation must be solved numerically for each material composition to obtain the eigenvalues and eigenvectors that give the resulting field quantities. The focus of this work was the development of a technique to obtain a closed form solution for the electromechanical crack tip fields in piezoelectric materials using an orthotropy rescaling technique in which the coordinate system is rescaled based on the ratios of certain elastic, dielectric, and piezoelectric coefficients to reduce the governing field equations to the biharmonic equation. Solutions for an isotropic linear elastic material can then be utilized to obtain solutions for the anisotropic piezoelectric material. This leads to closed form solutions for the fields in terms of ratios of the elastic, dielectric, and piezoelectric coefficients. Orthotropic rescaling and the Stroh formalism are shown to yield the same crack tip fields for certain ratios of material constants and to differ for others. The results are compared and recommendations are made for when and when not to use the orthotropic rescaling approach. The results of this investigation will appeared in, W.S. Oates, C.S. Lynch, *"Orthotropic rescaling for crack tip fields in linear piezoelectric materials"*, <u>International Journal of Solids and Structures</u> **41** (11-12) pp 2899-2917 (2003). This paper was also presented at the 2003 SPIE Smart Structures and Materials Conference and won a Best Student Paper Award.

In 2003, C.M. Landis was invited to submit a review paper on phenomenological constitutive modeling of ferroelectric ceramics. The contents of this review include work supported by this grant. The topics covered in the review are commensurate with the goals of the constitutive modeling phase of this research program. The abstract of the review article is as follows. "Due to the large coupling between their electrical and mechanical properties, ferroelectric ceramics are increasingly being implemented in novel devices. This review reports on recent advances in the development of predictive constitutive models for the coupled and nonlinear electromechanical behavior of ferroelectrics. Such constitutive models are required to analyze the performance of ferroelectric devices and to model the failure processes in these devices and materials. The topics covered in this review include micro-electromechanical constitutive models, macroscopic phenomenological modeling for polycrystals, and the implementation of these nonlinear constitutive models." This article appeared in, C.M. Landis, 2004. "Nonlinear Constitutive Modeling of Ferroelectrics", *Current Opinion in Solid State and Materials Science*, **8**, 59-69.

The work performed on this research project at Rice University heavily involved Prof. Landis' graduate student Jianxin Wang. Mr. Wang's work focused on the development and implementation of phenomenological constitutive laws for ferroelectric ceramics. These constitutive laws are electromechanically coupled, three dimensional (i.e. multi-axial), and can be integrated relatively quickly in comparison to micro-electromechanical models. Furthermore, these constitutive laws are able to predict a wide range of experimental observations and have been tested against more detailed micro-models. In fact, constitutive information obtained from the micro-models is incorporated directly into the phenomenological theory. In order to implement these constitutive laws within finite element codes, accurate backward Euler integration routines were developed. This step in the research program was not a trivial task as three forms of the backward Euler integration are required or useful. To explain, the constitutive law relates the histories of stress, strain, electric field and electric displacement to one another. The histories of one of the mechanical variables and one of the electrical variables must be given as input and the histories of the remaining variables are produced as output from the theory. Hence there are four possible forms of the constitutive integration. The first form that is useful for comparing the theory to experimental observations uses the stress and electric field histories as input and yields the strain and electric displacement as output. The second form that is required for fracture simulations with electric field and remanent polarization parallel to the crack front takes the strain and electric field histories as input and gives stress and electric displacement as output. Finally, the form that is required for fracture simulations with in-plane electric fields and for the vector potential finite element formulation of Landis (*IJNME* 2002) takes strain and electric displacement as input and gives stress and electric field as output. All three of these constitutive integration forms have been coded and thoroughly tested.

The constitutive integration routine described above has been implemented in a finite element code to investigate the effects of out-of-plane electric field on the

steady-state toughness enhancement due to domain switching in ferroelectric ceramics. Mode I steady crack growth is analyzed to determine the toughening due to domain switching in ferroelectric ceramics with electric field applied parallel to the crack front. The electromechanically coupled incremental constitutive theory developed previously in this research program is applied to model the material behavior of the ferroelectric. The constitutive law is then implemented within the finite element method to study steady crack growth. The toughening effects of electric field on both initially unpoled and poled materials are investigated. Results for the predicted fracture toughness, remanent strain and remanent polarization distributions, and domain switching zone shapes and sizes are presented. The effects of the plane-strain constraint and transverse stress are also established. The results of this study have uncovered some very interesting behaviors. Of considerable importance is the fact that the out-of-plane mechanical constraint plays a significant role in the fracture toughness of these materials, a prediction of the model that is confirmed by experimental observations. Other predictions of the model do not yet have corresponding experimental verification or refutation, and hence suggest new experimental studies. Details of this work were published in, J. Wang and C.M. Landis, 2004. "On the Fracture Toughness of Ferroelectric Ceramics with Electric Field Applied Parallel to the Crack Front", *Acta Materialia,* **52**, 3435-3446.

A phase field model that accounts for domain formation and evolution in ferroelectric materials under electro-mechanical loading was developed using the time-dependent Ginzburg-Landau equations. This work was motivated by a need to understand material behavior of ferroelectric single crystals and ceramics at the sub-grain level to increase reliability in actuator and sensor applications. Ferroelectric materials are known to form regions of like polarization (domains) at the micro and nano level to reduce the depolarization energy. Each domain is separated by a domain wall. Experiments conducted on the ferroelectric relaxor PZN-4.5%PT have shown that cracks tend to form along domain walls from electrical and mechanical loading. The phase field model uses a minimization of global free energy to simulate the evolution of domain structures through the time-dependent Ginzburg-Landau equation. Work has focused on the assumptions made when setting up the free energy function and the effect of these assumptions on the behavior of the model. Polarization is used as the independent variable. A fourth order polynomial is used to create energy minima that represent the tetragonal phase. Linear superposition is used to modify the energy to account for the effects of stress, electric field, and polarization gradients. The domain wall motion resulting from the mechanical and electrical external loading has been illustrated in the simulations. These simulations show that the switching process occurs uniquely in the region of domain walls and near boundaries where the polarization field is less stable than within the domain.

Some attention was focused on modeling fracture behavior in ferroelectric ceramics and relaxor single crystals. Critical mechanisms causing fatigue crack growth from cyclic electric fields in the ferroelectric ceramic (PZT) were identified using finite element analysis. A linear thermo-electro-mechanical finite element model was developed to approximate how ferroelectric switching and piezoelectric

coupling contributes to the fracture process during bi-polar electric field loading. It was shown that inhomogeneous switching near the crack tip contributes to the driving force for crack propagation. Ferroelectric material in the wake of the crack is shielded by the dielectric fluid in the crack volume, which creates a potential drop across the crack face thus inducing a larger field in front of the crack tip. This creates residual stress from ferroelectric switching in front of the crack tip and less switching in the crack wake. By introducing thermal coupling, the mismatch in material that switches ahead of the crack and the material that does not switch in the crack wake was modeled. The weight function method was employed to show that the stress intensity factor increases due to the inhomogeneous switching behavior. This is believed to be a major source of electrical fatigue in ferroelectric ceramics.

In addition, theoretical analysis on the fracture behavior of unpoled and poled (1-x)Pb($Zn_{2/3}Nb_{1/3}$)-x$PbTiO_3$ (x=0.045) (PZN-4.5%PT) single crystal relaxor ferroelectrics was conducted. This was motivated by recent R-curve measurements conducted by graduate student, William Oates. PZN-4.5%PT contains strong crystal anisotropy and fracture behavior. It was observed that cracks tend to form and propagate along the [110] domain wall from four point bend experiments using V-Notched bend bars. The fracture toughness was much lower (~K_I=0.4 MPa) along this cleavage plane. By using an anisotropic elasticity technique (Stroh's formalism), the crack tip toughness and local / global energy release rates were determined. It was shown that the crack tip toughness closely matched the applied toughness on the weak cleave plane. The toughness was almost double that when cracks propagated along the [010] plane. This work was pubished in, Oates, William S.; Lynch, Christopher S.; Lupascu, Doru C.; Njiwa, Alain B. Kounga; Aulbach, Emil; Rodel, Jurgen "subcritical crack growth in lead zirconate titanate" *Journal of the American Ceramic Society*, v 87, n 7, July, 2004, p 1362-1364A

This ARO grant supported Jianxin Wang throughout the majority of his graduate studies. Dr. Wang successfully defended his PhD dissertation "Fracture toughening of ferroelectric ceramics under electro-mechanical loading" in the summer of 2006. The focus of his research was on the development of constitutive models for the non-linear electromechanical behavior for polycrystalline ferroelectric ceramics. He and Landis have developed a thermodynamically consistent phenomenological framework for the constitutive model. The primary inputs to the phenomenological model include a description of the switching surface in stress and electric field space, and a representation of the "hardening potential" in remanent strain and remanent polarization space. In many aspects the model is similar to associated flow theory plasticity with kinematic hardening. In addition to using experimental observations as fitting functions for the theory, micro-electromechanical simulations have also been applied in order to deduce "hardening potentials" that allow them to accurately predict when the saturation of remanent strain and polarization occurs in these materials. These simulations have enriched the phenomenological theory by providing insights that would be difficult if not impossible to obtain in the lab.

With the newly devised constitutive model in hand, the next task was to apply the model within the finite element method to investigate the effects of domain switching

on the fracture toughness of ferroelectric ceramics under mixed electrical and mechanical loading. The simulations that they were able to perform fall under the name of Non-Linear Piezoelectric Fracture Mechanics (NLPFM). These simulations were the first of their kind that were able to predict the inhomogeneous distribution and intensity of the remanent strain and remanent polarization within the domain switching zone near a steadily growing crack tip. These simulations were also able to explain experimental observations that were inexplicable by prior modeling approaches and also went against most researcher's intuitions about how toughening should be affected by initial polarization. Specifically, the result that the toughness enhancement due to domain switching for an unpoled material and a material poled parallel to the crack front are similar has been confirmed experimentally and can be explained by considering the effects of the plane strain constraint near the crack tip. Finally, the most recent results on the effects of in-plane polarization and electric field on the fracture toughness illustrate a wide range of behaviors and these results have been included in a paper that has been accepted for publication and will appear soon.

In the final phase of the project two codes were completed by Lynch and Liu, and constitutive laws implemented. This work has not yet been published and is thus summarized in this report in more detail than the other findings. The two codes include a scalar potential formulation and a vector potential formulation. The scalar potential formulation is outlined in figure 1. This formulation satisfies the generalized equilibrium equations in the form of zero divergence of the stress tensor and zero divergence of the electric displacement vector fields. The nodal degrees of freedom are the mechanical displacement components and the scalar potential for the electric field. Constant strain – constant electric field triangle elements are implemented in the code.

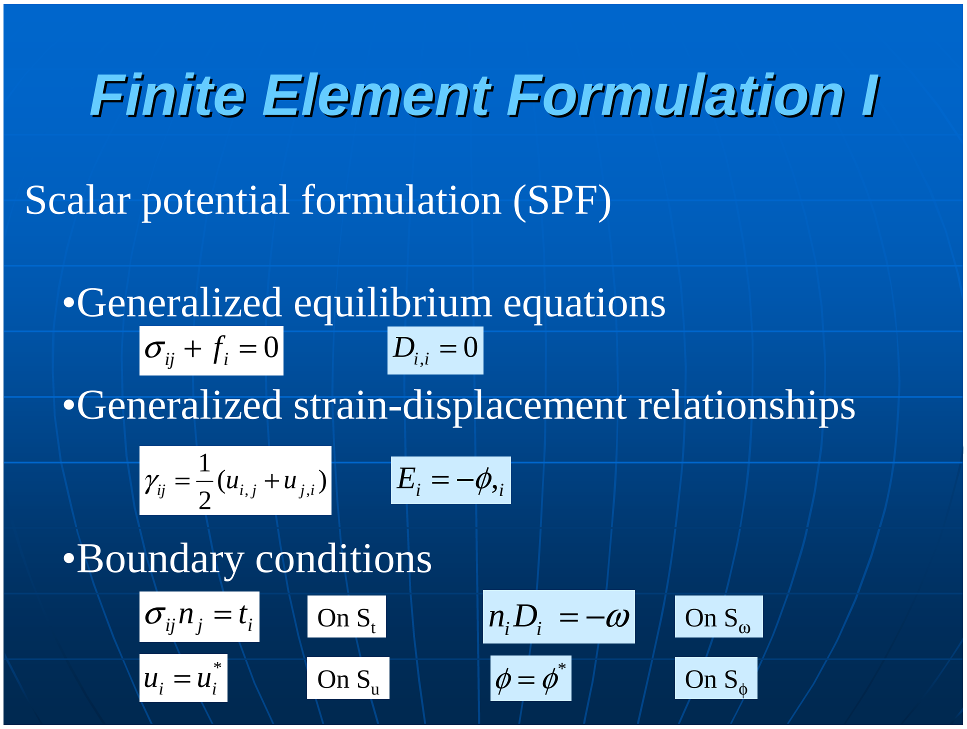


Figure 1. Outline of the scalar potential formulation.

The vector potential formulation satisfies the same equations, but in a different manner. In this case the condition of zero divergence of electric displacement is enforced through the introduction of a vector potential where the electric displacement is given by the curl of the vector potential. Since div(curl(psi))=0 is a vector identity, div(D)=0 is enforced. In this formulation the nodal degrees of freedom are the mechanical displacement and the vector potential. For the two dimensional formulation using constant strain and constant polarization triangle elements, only one component of the vector potential is required.

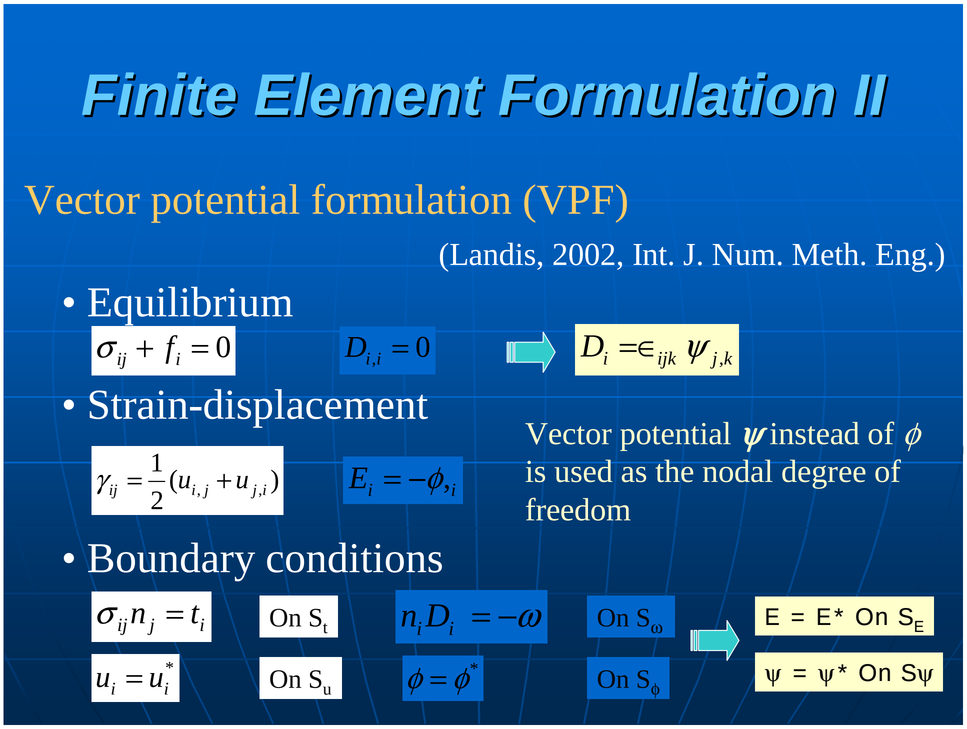


Figure 2. Outline of the vector potential formulation.

The two different formulations require different forms of the piezoelectric constitutive law, the stress-electric displacement form for the scalar potential formulation and the stress-electric field form for the vector potential form. In each case the constitutive law is a function of the remanent polarization and remanent strain. These terms enter the equations explicitly as seen in figure 3 through the direct calculation of the reversible strain and reversible electric displacement.

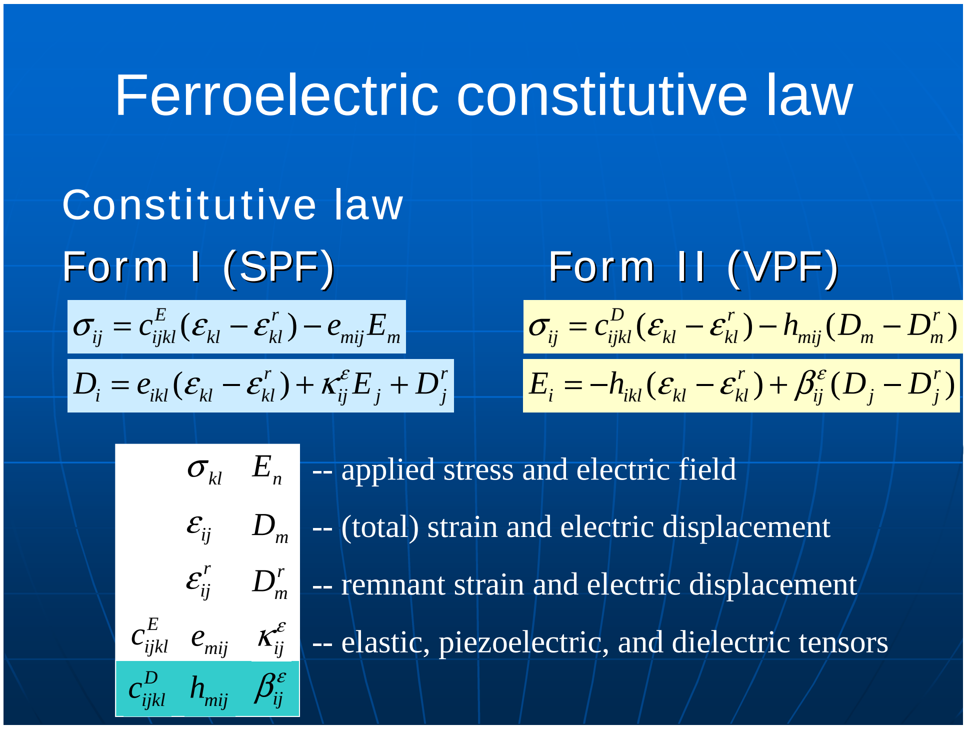


Figure 3. Outline of the linear piezoelectric constitutive laws implemented in the code.

In addition to the remanent terms entering the equations through the calculation of the reversible strain and polarization increments; the elastic, piezoelectric, and dielectric coefficients are all functions of the remanent strain and remanent polarization. The code is set up to solve boundary value problems through an incremental approach. The boundary conditions (electrical and mechanical loads) are applied in small steps. A linear finite element solution is found using a linear constitutive law. The stress and electric field at each element are then passed to a subroutine that handles the evolution of remanent strain and remanent polarization of each element through a micromechanics constitutive law that utlized a switching criterion as outlined in Figure 4. The new values of remanent strain and remanent polarization are then used to update the linear constitutive law of each element and the finite element solution is re-calculated. This process is repeated until convergence, and then the applied loads are incremented.

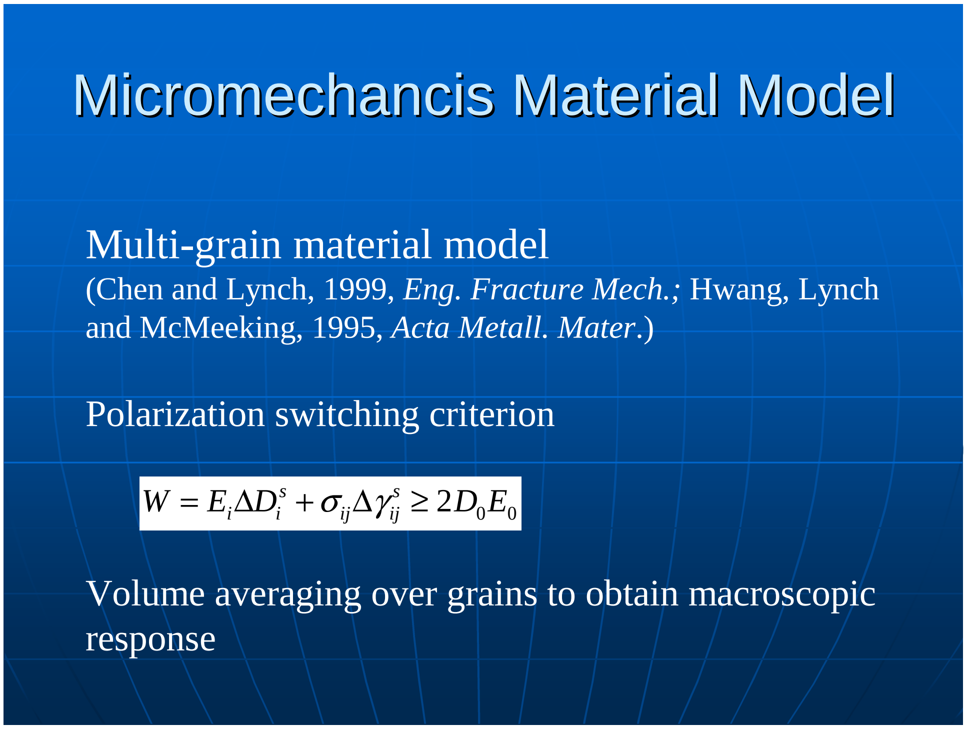
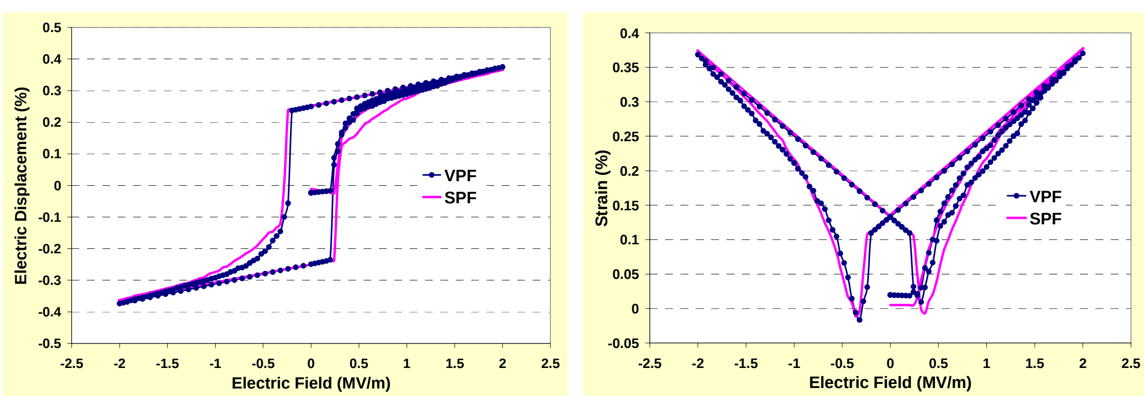


Figure 4. Outline of the micromechanics based switching criterion implemented in the finite element code.

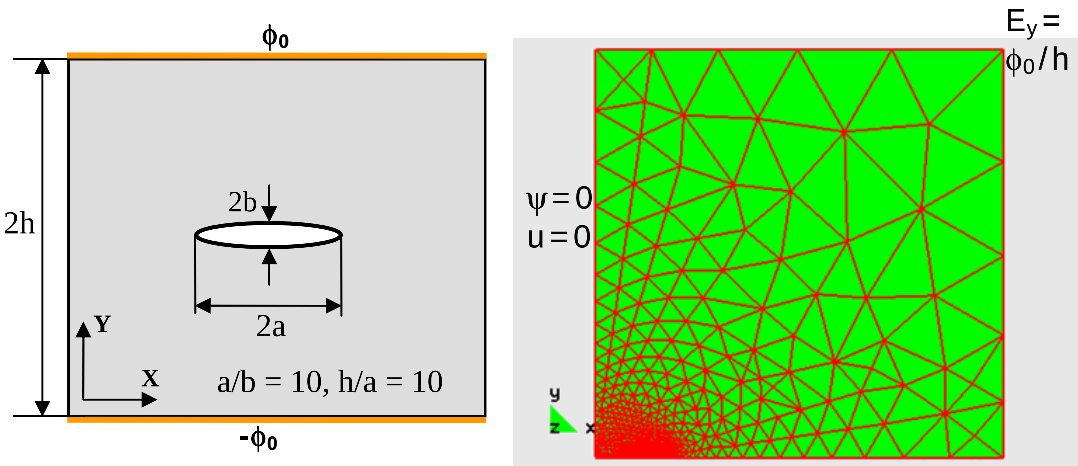
Examples of the capability of the finite element code that was developed under this research program are presented below. Figure 5 is a demonstration that the code is capable of simulating major hysteresis loops. In this simulation a solid rectangular block of material was meshed, assigned material properties, and subjected to a cyclic electric field.



(a) (b)

Figure 5. Finite element simulation of electric field induced polarization switching. (a) Strain response and (b) electric displacement response under uniform electric field. VPF and SPF give similar results. The difference is mainly due to the different grain sets used in the two simulations.

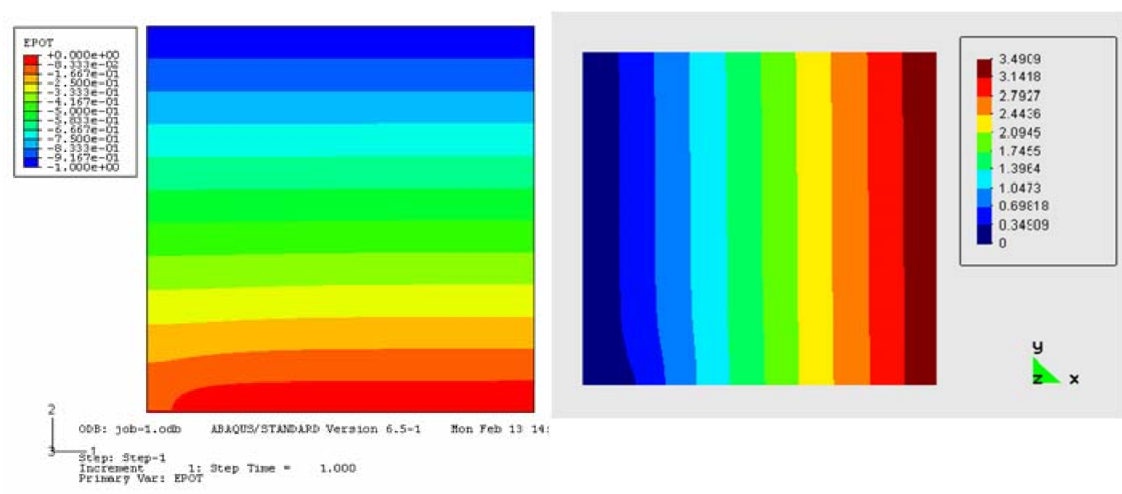
Figure 6 shows the geometry used in a simulation of a through crack (a slender ellipse). A quarter of the geometry shown in Figure 6 (a) is used in the finite element analysis. According to the symmetry, displacement component u=0 is applied at the left side and v=0 is applied at the bottom side. For the vector potential formulation, the electric displacement vector potential ψ=0 is given at the left side. For the scalar potential formulation, the electric field E_y= ϕ_0/h is applied at the top side as step loadings.



(a) (b)

Figure 6. Analysis of a through crack. (a) The physical model; (b) finite element mesh and boundary conditions. The void is treated as air with a dielectric permittivity of free space.

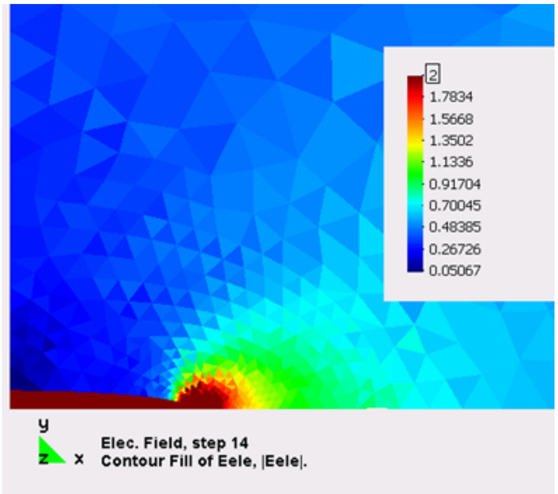
In the finite element calculations the load is incremented in steps. Figure 7 shows plots of (a) the scalar potential and (b) the vector potential once the loading has reached a peak value.



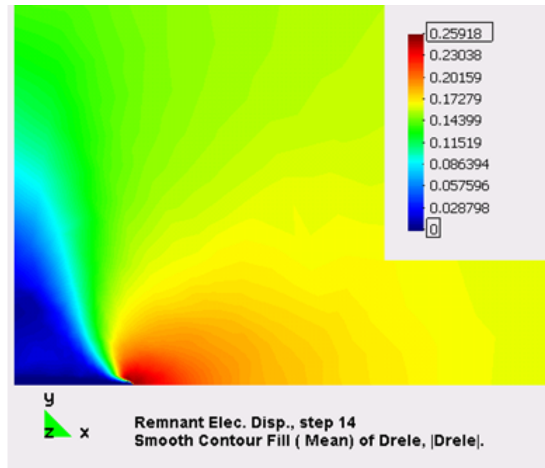
(a) (b)

Figure 7. Scalar potential versus vector potential. (a) Scalar electric potential distribution; (b) electric displacement vector potential distribution.

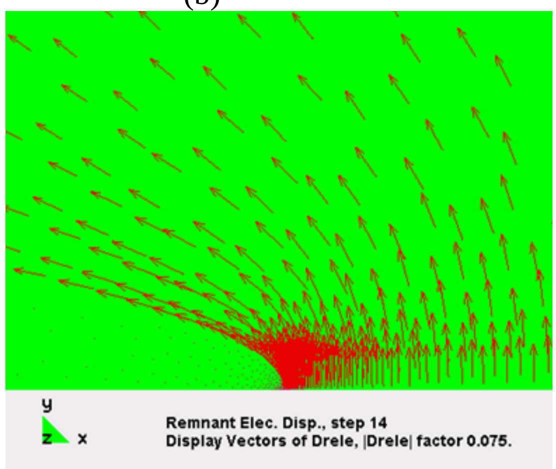
Figure 8 shows the a) electric field concentration, b) the remanent electric displacement distribution, and c) the remanent electric displacement direction induced by an elliptic through flaw.



(a)



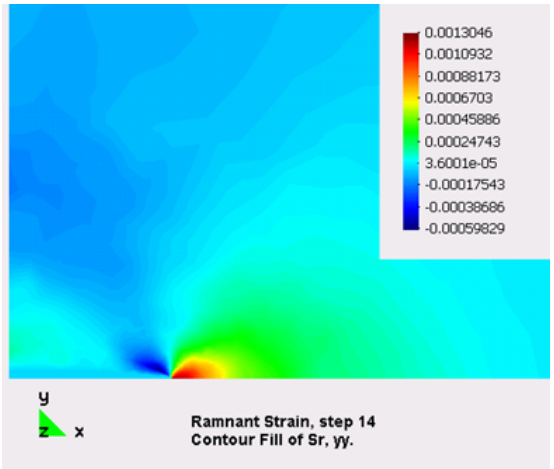
(b)

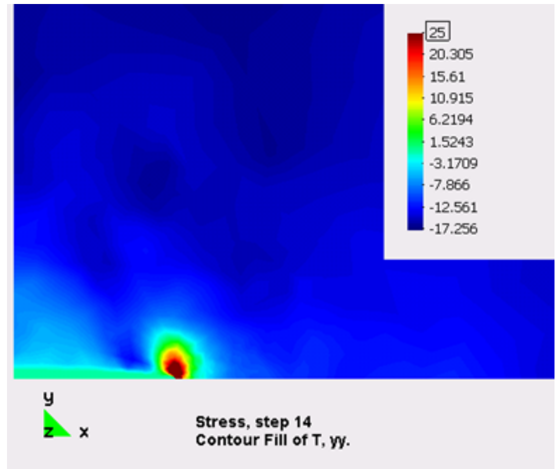


(c)

Figure 8. (a) Electric field and (b)(c) remnant electric displacement distribution at the crack tip. Remote field E_y= 0.5 MV/m.

Figure 9 shows the distribution of remanent strain and the local stress field generated by an applied electric field. The stress levels can be high enough to induce crack propagation

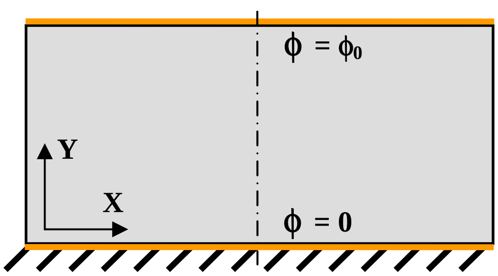


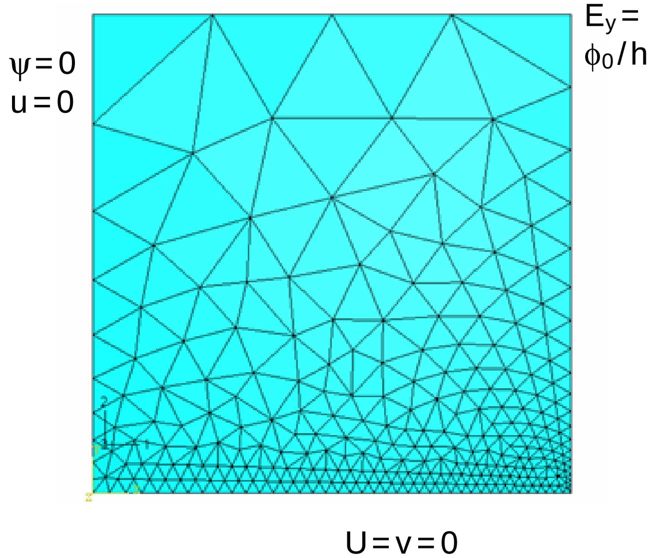


(a) (b)

Figure 9. Distribution of (a) remnant strain component ε_{22}^{r} and (b) stress component σ_{22} at the crack tip. Remote field E_y= 0.5 MV/m. Note that tensile stress σ_{22} is induced at the crack front during initial polarization as well as reverse polarization switching.

Figure 10 shows a second geometry that was simulated. This geometry represents the situation that occurs when a ferroelectric actuator material is bonded to a structure or to an end cap. Three of the surfaces are free. The bottom is fixed. Electric potential is applied at the top surface. The bottom is at zero potential.





(a) (b)

Figure 10. Rigid bonding on one end of the actuator. (a) The physical model; (b) finite element mesh and boundary conditions.

The results are shown in Figures 11 and 12. The ferroelectric material is poled in the vertical direction. This results in an extension in the vertical direction and contraction in the horizontal direction. The contraction is constrained at the bonding location. This induces a ferroelastic rotation of the polarization at this location, resulting in both an electric field concentration and a stress concentration.

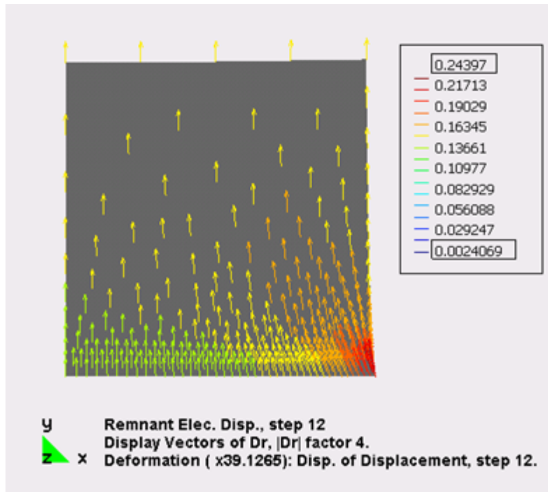
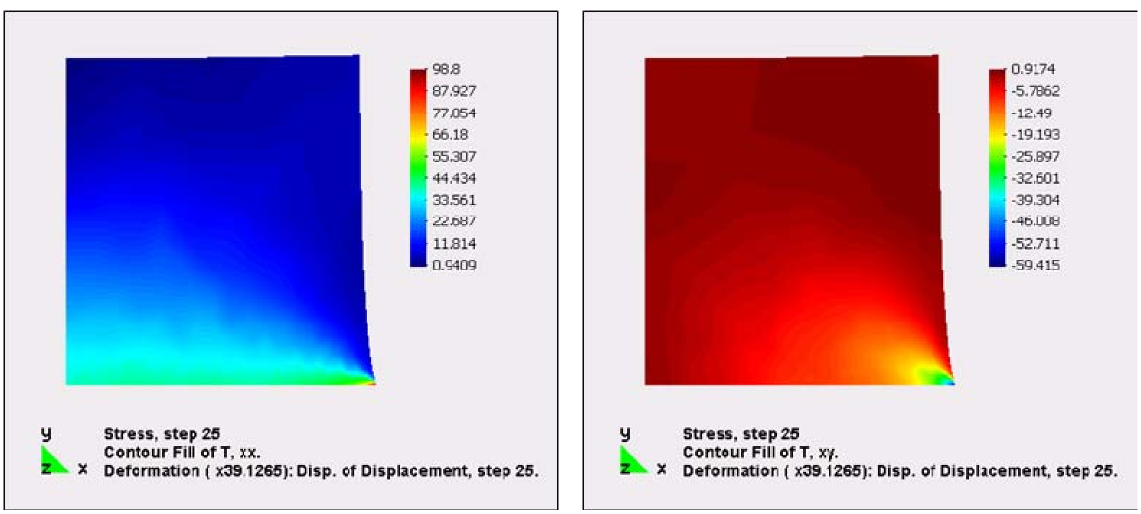


Figure 11. Remnant electric displacement distribution at initial polarization (deformed geometry). Applied field E_y = 0.5 MV/m.



(a) (b)

Figure 12. Stress distribution at applied field E_y = 1.0 MV/m (deformed geometry). (a) σ_{11}; (b) σ_{12}. There are also large tensile stress in y and z directions concentrated at the corner.

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